PHOTOCHEMICAL AND DISHARGE-DRIVEN PATHWAYS TO AROMATICS FROM 1,3-BUTADIENE: EXPLORING AROMATIC PRODUCTION IN TITAN'S ATMOSPHERE

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The dense haze observed on Saturn's moon Titan has been the source of much discussion and intrigue for many years. Recent models of Titan's atmosphere postulate that benzene is formed primarily in a two step process initiated by UV photodissociation of 1,3-butadiene to product propargyl + methyl, with propargyl radical recombination leading to benzene, much as it does in flames. Using a short reaction tube fixed to the end of our pulsed valve, we have studied the photochemical and discharge-driven pathways to aromatics under temperature and pressure conditions appropriate to Titan's atmosphere ($\sim$100 K and a few mbar). Photochemical production occurs while the reaction mixture is in the reaction tube, and then quenched $\sim$10 microsecond later as the mixture expands into vacuum. VUV or R2PI detection is used to detect the products formed, using time-of-flight mass detection. No benzene is photochemically produced under these cold-temperature conditions, while an abundance of benzene is formed with the electric discharge. The only observed aromatic products following photochemical excitation of 1,3-butadiene are 3-phenyl propyne and ethyl benzene, positively identified by their R2PI spectra. The discharge products were also interrogated by R2PI spectroscopy. Over 20 stable molecule and radical products were detected in this way, 16 of which are aromatics. The complex network of reaction products will be described, from which key reaction pathways are postulated.